201-16118

Chemtura Corporation
Benson Road 2-19
Middlebury, CT 06749
Regulatory Compliance

December 21, 2005

Administrator
ATTN: Chemical Right-to-Know Program
US Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Dear Sir or Madam: Re: Barium Stearate, CAS No. 6865-35-6

Chemtura Corporation is providing this letter and submission of a Test Plan and robust summaries as part of our commitment to sponsor CAS Number 6865-35-6 (Barium Stearate) under the HPV Challenge Program.

If you have any questions regarding our commitment, please feel free to contact me at (203) 573-2219 or Alan.Taylor@chemtura.com. You may also contact Dr. Wendy Koch, Epona Associates, LLC at (860) 429-0038 or wendykoch@eponallc.com.

Yours very truly,

Alan Taylor
Regulatory Compliance
Chemtura Corporation

Attachments: Test Plan
Appendices 1 and 2

cc Charles M. Auer, Director
Office of Pollution Prevention and Toxics
US EPA Headquarters
1200 Pennsylvania Avenue, N.W.
Mail Code: 7401M
Washington, DC 20460

BARIUM STEARATE (CAS NO. 6865-35-6): TEST PLAN

Submitted to the US Environmental Protection Agency

By

Chemtura Corporation

DATE: December 22, 2005

SUMMARY

Chemtura Corporation (Chemtura) has sponsored Barium stearate (CAS No. 6865-35-6) under the EPA's High Production Volume (HPV) Program. This document provides the Test Plan and summaries of existing data for this substance.

1.0 INTRODUCTION

Chemtura has voluntarily committed to participate in the Environmental Protection Agency's (EPA) high production volume chemicals (HPV) challenge program, to assess the health and environmental hazards, including selected physical chemical characteristics of barium stearate (CAS No. 6865-35-6).

An evaluation of the available data and proposed test plan are included in this document. As part of this evaluation, data from dissociation products was used to fulfill some endpoints for the sponsored substance. Robust summaries for barium stearate and dissociation products are provided in Appendix 1.

The objective of this test plan is to evaluate the available data and determine what additional data, if any, are needed to adequately characterize the physical properties, environmental fate, and human health and environmental effects of barium stearate. It is proposed that additional studies be conducted as shown in Table 1.

Table 1: AVAILABLE DATA FOR BARIUM STEARATE

Endpoint	
Physical Chemical Properties	
Melting Point	A
Vapor Pressure	Estimated/Not relevant*
Boiling Point	Estimated/Not relevant*
Partition Coefficient	Estimated/Not relevant** R (B,S)
Water Solubility	A
Environmental Fate	
Hydrolysis	Not relevant**
Photodegradation	A
Biodegradation	R (S)
Environmental Transport	A
Ecotoxicity	
Acute Fish	Not relevant*** R (B)
Acute Daphnia	Not relevant*** R (B,S)
Acute Algae	Not relevant*** R (B)
Chronic Daphnia	Test
Mammalian toxicity	
Acute Oral	A
Repeated Dose	R (B,S)
Genotoxicity (*in vitro* -bacteria)	R (B,S)
Genotoxicity (*in vivo*)	R (B,S)
Reproductive/Developmental	R (B)

A= Adequate data
Not relevant*= due to the solid nature of the substance
Not relevant**= the substance readily dissociates
Not relevant***= Based on the low water solubility of barium stearate, the estimated high partition coefficient for barium stearate and the high partition coefficient of stearic acid, a chronic daphnia test is proposed
R = Read across to dissociation products: B= barium/compounds, S= Stearic acid
Test = Testing is proposed
Estimated = Value calculated using EPIWIN

2.0 POTENTIAL USE AND EXPOSURE

Barium stearate is a solid material used as a lubricant/processing aid in PVC compounding.

3.0 EVALUATION OF EXISTING DATA AND PROPOSED TESTING

One key characteristic of barium stearate is that it readily dissociates from an ion pair into free metal and free acid. Barium stearate is found as a partially dissociated product in the ambient environment (i.e., neutral pH). Dissociation is a reversible process and the portion of dissociated salt present is dependent on the pH and pKa (the dissociation constant), which is the pH at which 50% dissociation occurs. In the low pH environment of the digestive tract (e.g., pH 1.2) complete dissociation will occur. The transport and bioavailability of the metals and acids are determined by their solubility in environmental media and biological fluids which is determined by environmental parameters such as pH.

Dissociation studies have been conducted for barium stearate and the results show that significant dissociation will occur at approximately neutral pH (i.e., representative of aquatic and marine ecosystems), while complete dissociation will occur at physiologically relevant pH of the mammalian stomach (pH 1.2) (Lezotte, F.J. and W.B. Nixon, 2002). These findings are particularly important in relating available data for the respective acids and metals to support the existing data and in the fulfillment of critical endpoints.

The dissociation constant is important for two reasons. First, it determines the proportion of any specific acid or metal that is dissociated at a given pH. The free acid and corresponding free metal are often much different than the salt (ion pair) moiety in characteristics such as solubility, adsorption, and toxicity. The proportion of dissociation influences the behavior of the substance in the environment and the bioavailablity of the acid and metal constituents of metal carboxylate salts.

The dissociation constant indicates that barium stearate has a pKa (pKb) values (pKa1) in the neutral range (6.706). This indicates that in the neutral pH range, significant portions of the metal carboxylate will be dissociated. In addition, at the low pH of the mammalian stomach (pH 1.2) all of the metal carboxylate would be expected to be completely or nearly completely dissociated. This indicates that the absorption and any observed toxicity would be independent for the respective acid and metal when administered orally.

The dissociation constants show that at the pH of the stomach and at the pH of environmental media the important moieties are the ionized free acid and metal. Because of this, data for environmental fate, ecotoxicity, and mammalian toxicity of the free acid, or that for a simple salt (e.g., the sodium salt), can serve as surrogate data for the acid component of respective metal carboxylates. Similarly, under these conditions, data for the metal ion can be represented by fate and toxicity data of free metal ion or simple metal salts (e.g., barium chloride). Therefore, the role in any observed toxicity for acids and metals can be evaluated independently (i.e., as the free metal and/or free acid).

In this test plan, the dissociation products [represented by barium (CAS No. 7440-39-3), barium chloride (CAS No. 10361-37-2) and barium sulfate (CAS No. 7727-43-7), as well as stearic acid (CAS No. 57-11-4)] are used to supplement the physical/chemical properties, environmental fate, aquatic toxicity and mammalian toxicity endpoints for barium stearate.

The available data have been assessed (see Tables 2 through 5). Robust summaries are provided as Appendix 1.

Chemical/Physical Properties:

Barium stearate is a solid. The determination of physical and chemical properties is limited by physical state (solid) and low water solubility. Physical chemical properties are provided in Table 2. The melting point of barium stearate is 160 °C (NISC BiblioLine, 2005). A boiling point has not been determined; the estimated boiling point is 661 °C (EPI SUMMARY, 2005). A vapor pressure has not been determined but it is expected to be negligible, and is not appropriate for determination. The modeled vapor pressure is $7.52E^{-14}$ mm Hg (0 hPa) (EPI SUMMARY, 2005). The physical and chemical properties of the dissociation products of barium stearate are also provided in Table 2. With the exception of barium chloride, the dissociation products of barium stearate have very low water solubility's.

Table 2: Summary of Physical and Chemical Property Data for Barium Stearate and Dissociation Products

Compound	Physical Chemical Properties			
	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Water Solubility
Barium stearate	160	* 661 Not relevant	* 0 Not relevant/ Negligible	3.5 mg/L at 20 °C
Dissociation products				
Barium	~710[2]	~1600[2]	*** Not relevant/ Negligible	*** Not relevant/ Negligible
Barium sulfate	1580[1] (decomposes)	1149[1]	*** Not relevant/ Negligible	Insoluble**[2]
Barium chloride	963[2]	1560[3]	*** Not relevant/ Negligible[3]	37.5 g/100 cm3 at 26 °C[4]
Stearic acid	69-70[5]	383[5]	1.33 at 174°C[6]	.568 mg/l at 25 °C[7]

* = Barium stearate is a solid; determination of boiling point and vapor pressure is not appropriate
** = 1 gram in 400,000 parts
*** = not relevant for metals/metal compounds

Recommendation: No additional testing proposed.

Environmental Fate:

The determination of partition coefficient, hydrolysis and biodegradation are not relevant for barium stearate due to its low water solubility and ready dissociation. As discussed above, barium stearate readily dissociates rather than hydrolyzing in water. Photodegradation and fugacity modeling has been conducted for barium stearate (EPI SUMMARY, 2005). The photodegradation half-life is 0.249 days. Level III fugacity modeling indicates barium stearate will partition primarily to soil and sediment.

Modeled partition coefficients for barium compounds are low (Table 3) (EPI SUMMARY, 2005). Hydrolysis of barium compounds is not relevant as they will dissociate and ionize in water. Photodegradation modeling cannot be conducted for these substances (EpiWin results are presented in Appendix 2). Level III fugacity modeling indicates distribution to soil and water for barium chloride and barium sulfate. Barium is expected to distribute primarily to air and water. For barium compounds, biodegradation is not expected to occur.

Stearic acid has a high partition coefficient (Leo, A.J., 1978) and low water solubility (Robb, ID, 1966) and is hydrolytically stable. Photodegradation modeling indicates a half-life of 0.5 days (EPI

1 ATSDR (1992)
2 O'Neil, MJ, Smith, A, Heckelman, PE and JR Obenchain (eds.) (2002)
3 Department of Health and Human Services, National Institute of Occupational Safety and Health (1990)
4 Http:/en.wikipedia.org/wiki/Barium Chloride (2005)
5 Windholz, M. (1982)
6 Weast, R.C. (1969)
7 Robb ID (1966)

SUMMARY, 2005). Fugacity modeling indicates distribution primarily to soil and sediment (EPI SUMMARY, 2005). Stearic acid is readily biodegradable (King, E.F.and Painter, H.A., 1983; Novak, J.T. and Kraus, D.L., 1973; Ruffo, C., Galli, E., Arpino, A., 1984; Urano, K. and Saito, M., 1985).

Table 3 Summary of Environmental Fate Data for Barium Stearate and Dissociation Products

Compound	Environmental Fate				
	Partition Coefficient	Stability in Water	Photodegradation	Level III Fugacity Model	Biodegradation
Barium stearate	** 15.4	**/****	$T_{1/2}$ = .249 days Overall OH Rate Constant = 42.9098 E-12 cm3/molecule-sec	Air 0.0807 Water 2.32 Soil 30.7 Sediment 66.9	***
Dissociation products					
Barium	** 0.23 (Epiwin)	**/****	**** Not relevant	Air 37.9 Water 55.8 Soil 6.18 Sediment 0.0944	***
Barium sulfate	** 0.63 (Epiwin)	**/****	**** Not relevant	Air 1.42e-006 Water 47.4 Soil 52.5 Sediment 0.091	***
Barium chloride	** 0.85 (Epiwin)	**/****	**** Not relevant	Air 9.42e-006 Water 46 Soil 53.9 Sediment 0.0906	***
Stearic acid	8.42	Stable	T ½ = .5 days Overall OH Rate Constant = 22.4804 E-12 cm3/molecule-sec	Air: 0.676 Water: 7.19 Soil: 28.9 Sediment: 63.3	= 77 % after 28 day(s)

** = Not relevant; substance readily dissociates
*** = Barium compounds are not expected to be readily biodegradable
**** = Can not be modeled with EPIWIN

Recommendation: No additional testing proposed.

Aquatic Toxicity

Aquatic toxicity data are not available for barium stearate. Data are available for barium and stearic acid, with 96 hr LC50 values in fish of >500 (Heitmuller, P.T., T.A. Hollister and P. R. Parrish, 1981) and 12 mg/l (Leach, J.M. and A.N. Thakore, 1977), respectively. The LC50 value (exposure period not specified) for barium chloride in fish is 42.7 mg/l (US EPA AQUIRE database, 2005). 48 hr LC50 values for daphnia are 68 mg/l (barium; LeBlanc, G.A.), 2.81 – 32 mg/l (barium sulfate; US EPA AQUIRE database, 2005; Khangarot BS and PK Ray, 1989) and 14.5 mg/l (barium chloride; Biesinger, KE and GN Christensen, 1972). The 96 hr EC50 value for algae is 25 mg/l (barium chloride; Wang, W, 1986). Aquatic toxicity data for daphnia and algae are not available for stearic acid.

Recommendation: Based on the low water solubility of barium stearate, the high predicted partition coefficient for barium stearate and the high partition coefficient of stearic acid, a chronic daphnia test is proposed.

Table 4 Aquatic Toxicity Data for Barium Stearate and Dissociation Products

Compound	Environmental Effects		
	96 hr LC50 Fish (mg/L)	48 hr LC50 Daphnia (mg/L)	96 hr EC50 Algae (mg/L)
Barium stearate	Not relevant*	Not relevant*	Not relevant*
Dissociation Products			
Barium	>500	410	Not available
Barium sulfate	LC0 = 59000	32 2.81	Not available
Barium chloride	42.7**	14.5	25
Stearic acid	12	Not available	Not available

Not relevant*= Based on the low water solubility of barium stearate, ready dissociation, and high partition coefficient of stearic acid, acute aquatic toxicity testing is not appropriate.
**Exposure period not specified

Acute Mammalian Toxicity:

Barium stearate has a low acute oral toxicity, with LD50's ranging from 2506 (Gigiena Truda i Professional'nye Zabolevaniya) to 3390 (Crompton Corporation, 2004) mg/kg (rat) and 1832 mg/kg (mouse) (Gigiena Truda i Professional'nye Zabolevaniya) (Table 5). Barium chloride has a much higher acute toxicity, most likely due to the higher water solubility, with values of 132 to >2000 (barium chloride dihydrate) mg/kg in rats (Tardiff, RG, M Robinson, NS Ulmer, 1980; National Toxicology Program, 1994) and >692 ppm (barium chloride dihydrate) in mice (National Toxicology Program, 1994). Stearic acid has a low acute oral toxicity, with an LD50 value of 4600 mg/kg (rat; Clayton, G.D., F.E. Clayton, 1993-1994).

Recommendation: No additional testing is proposed.

Repeated Dose Toxicity:

Repeated dose toxicity studies have not been conducted with barium stearate. However, both barium chloride and stearic acid have been tested. In a 13 week study of barium chloride dihydrate, rats received 125, 500, 1000, 2000 or 4000 ppm barium chloride in drinking water (National Toxicology Program, 1994). Three high dose males and one high dose female died during the last week of the study. Final mean body weights of the high dose group animals were significantly lower than controls. Water consumption at 4000 ppm was 30% lower than controls. There were no substance-related neurobehavioral, cardiovascular or clinical signs. Serum phosphorous levels were significantly higher than controls in both sexes in the 2000 and 4000 ppm groups. Renal tubule dilatation was observed in both sexes of the high dose group. The NOAEL was 1000 ppm. A 13 week study was also conducted in mice under the same protocol as described for rats above (National Toxicology Program, 1994). Six high dose males and seven high dose females died. One male in the 125 ppm group also died. Final mean body weights of the high dose group animals were significantly lower than controls. Water consumption was 18% lower than controls. Debilitation was observed in high dose animals. Absolute and/or relative liver weights were significantly lower in the 1000, 2000 and 4000 ppm group animals. Multifocal to diffuse nephropathy was observed in the high dose group. The NOAEL was 500 ppm. In a 13 week

drinking water study, rats were exposed to 10, 50 or 250 ppm barium chloride dihydrate (Tardiff, RG, M Robinson, NS Ulmer, 1980). Animals were sacrificed at 4, 8 and 13 weeks. No effects were observed for food consumption, clinical signs, body weight, hematology, serum enzymes, serum ions, gross pathology and histopathology. Water consumption was slightly decreased in the high dose animals. A slight decrease in relative adrenal weight was observed in treated animals versus controls. Increased dose resulted in increased concentrations in barium in liver, skeletal muscle, heart and bone. In a 14 day drinking water study, rats were exposed to 125, 250, 500, 1000 or 2000 ppm barium chloride (National Toxicology Program, 1994). There were no findings other than reduced water consumption at the high dose. The NOAEL was 1000 ppm. In a 14 day drinking water study, mice were exposed to 40, 80, 173, 346, 692 ppm barium chloride (National Toxicology Program, 1994). Increased relative and absolute liver weights were observed in high dose group animals. The NOAEL was 346 ppm.

Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue (Clayton, G.D., F.E. Clayton, 1993-1994). No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time. Rats fed 6% stearic acid for 9 weeks showed a decreased blood clotting time and hyperlipemia (Clayton, G.D., F.E. Clayton, 1993-1994). When diets containing 5 to 50% stearic acid (as the monoglyceride) were fed to weanling mice for 3 weeks, depression of weight gain was seen above the 10% dietary level (Clayton, G.D., F.E. Clayton, 1993-1994). Mortality occurred only with the 50% diet. The effects were less noticeable in adult mice.

Recommendation: No additional testing is proposed.

Reproductive/Developmental Toxicity:

Reproductive toxicity studies have not been conducted with barium stearate. A reproductive study has been conducted with barium chloride. Rats were exposed for 60 days prior to mating to 1000, 2000 or 4000 ppm barium chloride dihydrate in drinking water (WHO Environmental Health Criteria, 1990). There were no signs of reproductive or developmental toxicity. The NOAEL for reproductive or developmental toxicity was 4000 ppm. Mice were exposed for 60 days prior to mating to 500, 1000, or 2000 ppm barium chloride dihydrate in drinking water (WHO Environmental Health Criteria, 1990). There were no signs of reproductive or developmental toxicity. The NOAEL for reproductive or developmental toxicity was 2000 ppm.

There are no reproductive or developmental studies with stearic acid. However, stearic acid is the most common of the long-chain fatty acids. It is found in many foods, such as beef fat, and cocoa butter. It is widely used as a lubricant, in soaps, cosmetics, food packaging, deodorant sticks, toothpastes, and as a softener in rubber. Long-term safe use of this substance precludes the necessity for additional testing.

Recommendation: No additional testing is proposed.

Mutagenicity Assays:

No genetic toxicity testing is available for barium stearate. Barium chloride is negative for bacterial and mammalian genotoxicity (National Toxicology Program, 1994; Rossman, TG, M Molina, L Meyer, P Boone, CB Klein, Z Wang, F Li, WC Lin, and PL Kinney, 1991; National Toxicology Program, 1983). There are no mutagenicity assays with stearic acid. However, stearic acid is the

most common of the long-chain fatty acids. It is found in many foods, such as beef fat, and cocoa butter. It is widely used as a lubricant, in soaps, cosmetics, food packaging, deodorant sticks, toothpastes, and as a softener in rubber. Long-term safe use of this substance precludes the necessity for additional testing.

Recommendation: No additional testing is proposed.

Table 5 Mammalian Toxicity Data for Barium Stearate and Dissociation Products

Compound	Mammalian Toxicity				
	Oral LD50; (mg/kg)	Repeat Dose Toxicity	Repro. Effects	Develop. Effects	Genetic Toxicity
Barium stearate	3390 (rat) 2506 (rat) 1832 (mouse)	Not available	Not available	Not available	Not available
Dissociation Products					
Barium	Not available	Not available	Not available	Not available	Not available
Barium sulfate	Not available	Not available	Not available	Not available	Not available
Barium chloride	132 (rat) >2000 (rat) >692 ppm (mouse)	NOAEL = 1000 ppm (13 week, rat, drinking water) NOAEL = 500 ppm (13 week, mouse, drinking water) NOAEL = 1000 ppm (14 d, rat, drinking water) NOAEL = 346 ppm (14 d, mouse, drinking water) NOAEL = 50 ppm (13 week, rat. Drinking water) NOAEL = 209 (10 d, rat, drinking water) LOAEL = 100 mg/l (16 month, rat, drinking water)	NOAEL = 4000 mg/l (rat, drinking water) NOAEL = 2000 mg/l (mouse, drinking water)	NOAEL = 4000 mg/l (rat, drinking water)	Negative (bacterial mutation; in vitro chromosome aberration)
Stearic acid	4600 (rat)	50 g/kg/d for 24 weeks produced reversible lipogranulomas in rats. 6% for 9 weeks produced decreased blood clotting time and hyperlipemia in rats. NOAEL = 5% for 3 weeks (mice)	Not available	Not available	Not available

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1. General Information

ID 10361-37-2

Date 9 Nov 2005

1.0 SUBSTANCE INFORMATION

Generic Name	:	Barium chloride
Chemical Name	:	Barium dichloride
CAS Registry No.	:	10361-37-2
Component CAS Nos.	:	
EINECS No.	:	233-788-1
Structural Formula	:	$BaCl_2$
Additional description	:	
Molecular Weight	:	208.23
Synonyms and Tradenames	:	Barium (II) chloride; RTECS CQ8750000; HSDB 2633; NCI C61074
	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)
References		O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ. (molecular weight value)

2.1 MELTING POINT

Value	:	= 963 °C
Decomposition	:	
Sublimation	:	
Method	:	Other
Year	:	2002
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Source is well established data compendium.
Reference	:	O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ.

2.2 BOILING POINT

Value	:	= 1560 °C
Decomposition	:	
Method	:	Other
Year	:	1990
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Source is well established NIOSH reference.
Reference	:	Department of Health and Human Services, National Institute for Occupational Safety and Health. 1990. NIOSH Pocket Guide to Chemical Hazards. U.S. Government Printing Office, Washington, DC.

2.3 DENSITY

Type	:	density
Value	:	= 3.86 g/cm^3
Method		Other
Year	:	2002
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Source is well established data compendium.
Reference	:	O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ.

2.4 VAPOUR PRESSURE

Type	:	
Value	:	
Decomposition	:	
Method	:	Other
Year	:	1990
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	Low based on melting point and boiling point data
Reliability	:	(2) valid with restrictions Source is well established NIOSH reference.
Reference	:	Department of Health and Human Services, National Institute for Occupational Safety and Health. 1990. NIOSH Pocket Guide to Chemical Hazards. U.S. Government Printing Office, Washington, DC.

2.5 PARTITION COEFFICIENT

Type	:	
Partition coefficient	:	
Log Pow	:	
pH value	:	
Method	:	Other
Year	:	2005
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	Compound dissociates and ionizes in water
Reliability	:	(2) valid with restrictions Information taken from a secondary literature source (electronic database)
Reference	:	http://en.wikipedia.org/wiki/Barium_chloride (accessed 18 Oct. 2005)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 37.5 other: g/100 cm^3 at 26 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
PKa	:	at °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	Other
Year	:	2005
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Data taken from a secondary literature source (electronic database)
Reference	:	http://en.wikipedia.org/wiki/Barium_chloride

(accessed 18 Oct. 2005)

Solubility in	:	Water
Method	:	Other
Year	:	2002
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	Very soluble in water
Reliability	:	(2) valid with restrictions Source is well established data compendium.
Reference	:	O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ.

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Year	:	2005
Test substance	:	As prescribed by 1.1-1.4
Method	:	EPIWIN
Result	:	Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	9.42e-006	1e+005	1000
Water	46	900	1000
Soil	53.9	900	1000
Sediment	0.0906	3.6e+003	0

Persistence Time: 813 hr

Reliability	:	(2) valid with restrictions Data were obtained by modeling.
Reference	:	EPIWIN (ver 3.11) (2005)

3.3.2 DISTRIBUTION

3.5 BIODEGRADATION

4.1 ACUTE TOXICITY TO FISH

Type	:	Flow-through
Species	:	Rainbow trout (*Onchorhynchus mykiss*)
Exposure period	:	
Unit	:	ug/L
NOEC	:	
LC0	:	
LC50	:	= 42,700
LC100	:	
Limit test	:	
Analytical monitoring	:	No
Method	:	other
Year	:	1980
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Donaldson trout were used in the study.
Result	:	Slight toxicity in Rainbow trout, but determined not to be acutely toxic
Remark	:	The bioavailability and resultant aquatic toxicity of barium chloride are affected by a variety of factors, including water hardness, pH, dissolved organic carbon and temperature. Average reported LC_{50} values for barium chloride for various species of fish include 1,000,000 µg/L in eight studies of Mummichog (*Fundulus heteroclitus*) and 2,036,667 µg/L in three studies of Western mosquitofish (*Gambusia affinis*) and 870,000 µg/L in one study of Carp (Leuciscus idus melanotus) and 150,000 µg/L in one study of Brown trout (*Salmo trutta*) and four studies of Coho salmon (*Onchorhynchus kisutch)* using static exposures ranged from a 3 day NOEC of 88,800 µg/L to a 6 day NOEC of 282,000 µg/L (data derived from U.S. EPA, AQUIRE database, 2005)
Reliability	:	(2) valid with restrictions Insufficient details are present to indicate whether all test methods followed the Guidelines. However, methods and number of studies with similar results seem sufficient to accept the data
Reference	:	http://www.pesticideinfo.org/List_AquireAcuteSum.jsp?Rec_Id=PC35604&Taxa_Group=Fish) (accessed on 11/19/2005).

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	Flow-through
Species	:	*Daphnia magna* (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	ug/L
LC50	:	= 14,500
Limit test	:	
Analytical monitoring	:	
Method	:	other
Year	:	1972
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4

Result	:	LC50 = 14,500 µg/L (without food)
Remark	:	The bioavailability and resultant aquatic toxicity are affected by a variety of factors, including water hardness, pH, dissolved organic carbon and temperature. Several crustacean studies were found including two studies conducted in 1988 in Yellow Rock Crab (*Cancer anthonyi*) showing embryo toxicity after 7 days in flow-through studies at concentrations of 10,000 and 100,000 µg/L, respectively. Slight toxicity was seen in several Crayfish (*Austropotamobius pallipes pall*) studies conducted in 1973 in a static system. (U.S. EPA, AQUIRE database, 2005).
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	Biesinger, K. E. and G. N. Christensen. 1972. Effects of Various Metals on Survival, Growth, Reproduction, and Metabolism of *Daphnia magna*. J. Fish. Res. Bd. Canada, 29:1691-1700. http://www.pesticideinfo.org/List_AquireAll.jsp?Rec_Id=PC35604&Taxa_Group=Crustaceans (AQUIRE database info accessed on 11/9/05)

4.3 TOXICITY TO AQUATIC PLANTS (E.G., ALGAE)

Species	:	Other algae: Duckweed (*Lemna minor*)
Endpoint	:	Growth rate
Exposure period	:	96 hrs
Unit	:	ug/L
EC50	:	= 25,000
Limit test	:	
Analytical monitoring	:	
Method	:	other
Year	:	1986
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Static test
Remark	:	The bioavailability and resultant aquatic toxicity are affected by a variety of factors, including water hardness, pH, dissolved organic carbon and temperature The reported minimum toxic dose in aquatic moss (*Physcomitrella patens*) was 208.2 µg/L in studies published in 1990 and 1993 according to ASTM STP 1179 and 1091. (U.S. EPA, AQUIRE database, 2005). Reagent grade barium chloride was moderately toxic in de-ionized water and nontoxic in Illinois river water to Duckweed (Wang)
Reliability	:	(2) valid with restrictions. Comparable to guideline study
Reference	:	Wang, W. (1986) The Effect of River Water on Phytotoxicity of Ba, Cd and Cr. Environ. Pollut. Ser. B 0143-148. (as cited in AQUIRE data base accessed 10/19/05)

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

In vitro/in vivo	:	
Type	:	
Species	:	
Number of animals	:	

Males	:	
Females	:	
Doses	:	
Males	:	
Females	:	
Vehicle	:	
Route of administration	:	
Exposure time	:	
Product type guidance	:	
Decision on results on acute tox. tests	:	
Adverse effects on prolonged exposure	:	
Half-lives	:	1st: bone Estimated to be about 50 days 2nd: 3rd:
Toxic behavior	:	
Deg. product	:	
Deg. products CAS#	:	
Method	:	Other
Year	:	2005
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Remark	:	Human and animal studies suggest that barium chloride and other soluble barium salts administered orally, by injection or intragastrically are rapidly absorbed from the intestinal tract into the bloodstream and then into the muscle, lungs and bone with very little being retained by the soft tissues (with the exception of the eye). Fasted animals showed increased absorption of barium compounds (20% vs. 7%) than those with access to food. Barium compounds are generally absent from the blood within 24 hours, but retention in the bone is similar to calcium with a half-life estimated at 50 days. Approximately half the dose is bound to protein. These compounds are known to stimulate striated, cardiac and smooth muscle by displacing calcium in cell membranes which increases membrane permeability. Barium compounds activate secretion of catecholamines. Death may be caused by failure of muscular contractions resulting in respiratory failure and cardiovascular collapse. Non-lethal doses in rats were largely excreted in the feces (20%) and to a lesser extent in the urine (7%) within the first 24 hours. Barium clearance is increased by intravenous administration of saline solutions.
Test substance	:	Barium chloride and other soluble barium salts
Reliability	:	(2) valid with restrictions Summary based on peer-reviewed publications
Reference	:	Hazardous Substances Data Bank http://toxnet.nlm.nih.gov (accessed 8/16/05) //risk.lsd.ornl.gov/tox/profiles/barium_f_V1.shtml#te (accessed 11/9/2005)
In vitro/in vivo	:	In vivo
Type	:	Absorption
Species	:	Syrian hamster
Number of animals	:	
Males	:	

Females	:	
Doses	:	
Males	:	
Females	:	
Vehicle	:	
Route of administration	:	Inhalation
Exposure time	:	4 hour(s)
Product type guidance	:	
Decision on results on acute tox. tests	:	
Adverse effects on prolonged exposure	:	
Half-lives	:	1st: 2nd: 3rd:
Toxic behavior	:	
Deg. product	:	
Method	:	other
Year	:	
GLP	:	No
Test substance	:	Other TS
Remark	:	Nasopharynx was the major absorption site for inhaled aerosols of soluble barium, especially for readily soluble aerosols having a mass medium aerodynamic diameter of > 5 µm. Year of study unknown, but cited in 1990
Result	:	Barium absorption into the general circulation from nasal passages was approximately 61% as compared to 11% from GI absorption after four hours
Test substance	:	Labeled barium chloride
Reliability	:	(2) valid with restrictions Summary cited in peer-reviewed WHO report
Reference	:	WHO Environmental Health Criteria 107, Barium (1990)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50l
Value	:	= 132 mg/kg bw
Species	:	Rat
Strain	:	No data
Sex	:	Male/female
Number of animals	:	80
Vehicle	:	Water
Doses	:	Other: Not specified
Method	:	other
Year	:	1980
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Single dose administered by gavage (10 per dose level)
	:	Adult (60-70 days of age) and weanling (21-25 days of age) were used to determine the LD50 using BaCl2 dissolved in distilled water and administered by gavage. All animals were observed for 14 days.
Result	:	220 mg/Kg (500 mg BaCl2/Kg) in weanling rats (confidence limits 434-600) 132 mg/Kg (300 mg BaCl2/Kg) in adults (confidence limits 255-369). The

		results were used to select the dose for subchronic studies (Tardiff, et al.)
Remark	:	Acute LD50 values in rats ranged from 118-500 mg/Kg, 7-29 mg/Kg in mice, 90 mg/Kg in dogs, 170 mg/Kg in rabbits and 800-1200 mg/Kg in horses (Friberg, et al. 1986) Acute oral toxicity in humans is reported to occur at 80 mg/Kg (McCauley, et al. Chapter XVIII, page 197-210, book unknown)
Reliability	:	(2) valid with restrictions References from peer-reviewed publication
Reference	:	Friberg cited in Hazardous Substances Data Bank http://toxnet.nlm.nih.gov (accessed 8/16/05) Tardiff, R.G., M. Robinson, N. S. Ulmer. (1980) Subchronic Oral Toxicity of BaCl2 in Rats. J. Environ. Path. Toxicol. 4:267-275.

Type	:	LD50
Value	:	> 2000 ppm
Species	:	Rat
Strain	:	Other: F344/N
Sex	:	Male/female
Number of animals	:	
Vehicle	:	Water
Doses	:	
Method	:	other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Remark	:	NTP probably followed GLP criteria during that time.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Adequate documentation available in a study conducted by NTP.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	LD50
Value	:	>692 ppm
Species	:	Mouse
Strain	:	B6C3F1
Sex	:	Male/female
Number of animals	:	
Vehicle	:	Water
Doses	:	
Method	:	other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Remark	:	NTP probably followed GLP criteria during that time
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Adequate documentation available in a study conducted by NTP.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Remark	:	Not expected to cross intact skin due to the high polarity of the various forms of barium compounds most commonly encountered
Reliability	:	
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

5.2.1 SKIN IRRITATION

Remark	:	May be a human skin irritant, but no studies were found as confirmatory
Reliability	:	
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

5.2.2 EYE IRRITATION

Species	:	Rabbit
Concentration	:	
Dose	:	Other: 0.08 to 0.1 M solution
Exposure time	:	
Number of animals	:	
Vehicle	:	
Classification	:	
Method	:	Other
Year	:	1986
GLP	:	No data
Test substance	:	As prescribed by 1.1-1.4
Method	:	0.08 to 0.1 M solution injected into cornea (single injection); 10 minute dropping on eye after corneal epithelium was removed
Result	:	No opacification of cornea, but caused considerable iritis which subsided in a few days
Reliability	:	(3) invalid Non-standard method and few experimental details
Reference	:	Grant, W.M. (1986) Toxicology of the Eye. 3rd Edition. Springfield: Charles C. Thomas Publisher, p. 134

5.4 REPEATED DOSE TOXICITY

Type	:	Subchronic
Species	:	Rat

Strain	:	Other: F344/N
Sex	:	Male/female
Number of animals	:	
Route of admin.	:	Drinking water
Exposure period	:	13-Weeks
Frequency of treatment	:	Continuous
Post exposure period	:	None
Doses	:	125, 500, 1,000, 2,000 or 4,000 ppm corresponding to average daily doses of 10, 30, 65, 110 or 200 mg barium/kg/body weight in males and 10, 35, 65, 115 or 180 mg barium/kg/body weight in females
Control group	:	Yes, concurrent vehicle
NOAEL	:	
LOAEL	:	
Method	:	Other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Method	:	10 per sex per dose level; Measurements included body weights, water consumption, clinical signs, hematology and clinical chemistry, neurobehavioral effects, major organ pathology
Result	:	Three males and one female died in the high dose group in the last week of the study. Final mean body weights in high dose group in both sexes were significantly lower than controls. Water consumption at 4,000 ppm was 30% lower than controls. No clearly related chemical effects were noted in neurobehavioral, cardiovascular or clinical signs. Serum phosphorus levels were significantly higher than controls in box sexes at 2,000 and 4,000 ppm. Renal tubule dilatation in the outer stripe of the medulla and cortex occurred at the 4,000 ppm group in males and females.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.
Type	:	Sub-chronic
Species	:	Mice
Strain	:	B6C3F1
Sex	:	Male/female
Number of animals	:	
Route of admin.	:	Drinking water
Exposure period	:	13 wk
Frequency of treatment	:	Continuous
Post exposure period	:	None
Doses	:	125, 500, 1,000, 2,000 or 4,000 ppm corresponding to average daily doses of 15, 55, 100, 205 or 450 mg barium/kg body weight to males and 15, 60, 110, 200 or 495 mg barium/kg body weight in females
Control group	:	Yes, concurrent vehicle
NOAEL	:	
LOAEL	:	
Method	:	Other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS

5. Toxicity

ID 10361-37-2

Date 9 Nov 2005

Method	:	Groups of male and female rats (10 per sex per dose level) were given drinking water barium chloride dihydrate for 13 weeks. Animals were observed daily for clinical signs of toxicity and weighed weekly. Water intake was measured. Prior to study termination, blood samples were collected and analyzed for hematological and biochemical parameters. Following necropsy, gross pathological and histopathological examinations were conducted on selected target organs and tissues. Organs weights were also determined.
Results	:	Mortality was observed in six males and seven females at 4,000 ppm and in one male at 125 ppm. Final mean body weights at 4,000 ppm were significantly reduced (>30%) from controls. Water consumption was 18% lower than controls in males at 4,000 ppm while other doses were similar. Debilitation was observed in the surviving animals at 4,000 ppm. Absolute and/or relative liver weights in the 1,000, 2,000 and 4,000 ppm dose groups were significantly lower than controls. Multifocal to diffuse nephropathy characterized by tubule dilatation, regeneration and atrophy was observed in the high dose.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	Sub-acute
Species	:	Rat
Strain	:	Other: F344/N
Sex	:	Male/female
Route of admin.	:	Drinking water
Exposure period	:	14 days
Frequency of treatm.	:	continuous
Post exposure period	:	none
Doses	:	0, 125, 250, 500, 1,000 or 2,000 ppm
Control group	:	Yes, concurrent vehicle
Method	:	Other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Result	:	There were no findings in rats with the exception of decreased water consumption in high dose rats
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	Sub-acute
Species	:	Mouse
Strain	:	B6C3F1

Sex	:	Male/female
Route of admin.	:	Drinking water
Exposure period	:	14 days
Frequency of treatm.	:	continuous
Post exposure period	:	none
Doses	:	0, 40, 80, 173, 346 or 692 ppm
Control group	:	Yes, concurrent vehicle
Method	:	Other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Method	:	Daily in drinking water. Measurements of body weights, clinical findings, water consumption, hematology, clinical chemistry, relative/absolute organ weights and neurobehavioral patterns
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Result	:	There were no findings in mice with the exception of increased absolute and relative liver weights in high dose mice.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	Sub-chronic
Species	:	Rat
Strain	:	Charles River
Sex	:	Male/female
Number of animals	:	
Route of admin.	:	Drinking water
Exposure period	:	13 wk
Frequency of treatment	:	Continuous
Post exposure period	:	None
Doses	:	10, 50, or 250 ppm in drinking water (females had a slightly higher exposure to barium than males in all treatment groups)
Control group	:	Yes, concurrent vehicle
NOAEL	:	
LOAEL	:	
Method	:	
Year	:	1980
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Subgroups of at least 5 rats per sex per dose level were sacrificed at 4, 8 or 13 weeks for measurement of biochemical or hematologic parameters, comprehensive histopathological examination and analysis of barium levels in selected tissues. Water consumption was measured daily with weekly recording of body weights, food consumption and the presence of clinical signs. Animals were observed for mortality daily. All tissues were weighed and either frozen for analysis of barium concentration or histologic examination. Clinical chemistry and hematology measurements were made. Statistical analysis of organ weights, hematology and clinical chemistry variables were conducted.
Results	:	No adverse effects were observed for food consumption, clinical signs,

		body weight, hematology, serum enzymes, serum ions (Na, K, Ca), gross pathology and histopathology. Water consumption was slightly decreased in the high dose animals. A slight decrease in relative adrenal weight in treated animals was observed versus controls. Increased dose (but not exposure duration) resulted in increases in barium concentrations in liver, skeletal muscle, heart and bone with the highest concentrations observed in bone.
Remark	:	Two previous studies showed that barium was associated with an effect on adrenals altering the weight of the organ. Since barium results in the release of catecholamines from the adrenal medulla of cats and has a similar effect when bovine adrenals are perfused, the investigators postulated that barium acts on the chromatin cell membrane displacing calcium. Constant release of catecholamines results in depletion of intermediates and consequent atrophy.
Reliability	:	(2)valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	Tardiff, R.G., M. Robinson, N. S. Ulmer. (1980) Subchronic Oral Toxicity of BaCl2 in Rats. J. Environ. Path. Toxicol. 4:267-275.

Type	:	Sub-chronic
Species	:	Rats
Strain	:	Sprague-Dawley
Sex	:	Male/female
Number of animals	:	
Route of admin.	:	Drinking water
Exposure period	:	36, 46 or 68 weeks
Frequency of treatment	:	Continuous
Post exposure period	:	None
Doses	:	1, 10, 100, or 250 ppm Ba in drinking water for 36 weeks or 1, 10, or 100 ppm Ba for 68 weeks or 0 or 250 ppm Ba for 46 weeks
Control group	:	Yes, concurrent vehicle
NOAEL	:	
LOAEL	:	
Method	:	Other
Year	:	Unknown
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	This study utilized a number of non-standard measures and various dosing regimens. Animals were fed different diets with different levels of background barium present in the feed. 12 males per dose for 36 weeks; 10 males per dose for 68 weeks; 12 females per dose for 46 weeks
Results	:	There was a dose-related increase in retinal dystrophy and other studies do indicate that barium is absorbed in eye tissue. However, retinal dystrophy is a common degenerative disease in aging Sprague-Dawley rats and is affected by placement of lights and light penetration through plastic caging.
Remark	:	Results of this study are difficult to interpret due to the confounding factors presented above.
Reliability	:	(3) invalid Due to relevant methodological deficiencies
Reference	:	McCauley, et al. (year unknown) Chapter XVIII, page 197-210, photocopied from an unknown book

5.5 GENETIC TOXICITY - "IN VITRO"

Type	:	Ames test
System of testing	:	Salmonella typhimurium strains TA 97, TA 98, TA 100, TA 1535 or TA 1537
Test concentrations	:	Unknown
Cytotoxic concentr.	:	Not determined
Metabolic activation	:	With and without
Result	:	negative
Method	:	other
Year	:	1994
GLP	:	No data
Test substance	:	Other TS
Method	:	Not specified in summary report
Result	:	At the concentration tested, there was no indication of any mutagenic activity with or without exogenous metabolic activation
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Acceptable study with adequate documentation similar to Guideline study
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	
System of testing	:	Escherichia coli $WP_s(\lambda)$
Test concentrations	:	> 100 µg/well and 0.78 µg/well
Cytotoxic concentr.	:	
Metabolic activation	:	without
Year	:	1991
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Microscreen assay; Method of Rossman et al., 1984. Environ. Mut., 6:59.
Test substance	:	Reagent grade
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	Rossman, T.G., M. Molina, L. Meyer, P. Boone, C. B. Klein, Z. Wang, F. Li, W.C. Lin and P. L. Kinney. 1991. Performance of 133 compounds in the lambda prophage induction endpoint of the Microscreen assay and a comparison with S. typhimurium mutagenicity and rodent carcinogenicity assays. Mut. Res., 260:349-367.

Type	:	Mouse lymphoma assay
System of testing	:	Cultured mouse lymphoma cells – L5178/$TK^{+/-}$
Test concentrations	:	Not specified
Cytotoxic concentr.	:	Not determined
Metabolic activation	:	with and without
Result	:	Positive
Year	:	1994
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Method of Clive et al., 1972. Mutation Res., 16:77-87.

Result	:	Mutagenic in the presence of metabolic activation (S-9); negative without activation and equivocal in other assays with S-9 activation
Reliability	:	(2) valid with restrictions Acceptable study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Type	:	Chromosome aberration
System of testing	:	Mouse bone marrow cells
Test concentrations	:	50, 160, 500, 1,600 or 5,000 µg/mL
Cytotoxic concentr.	:	
Metabolic activation	:	With and without
Result	:	negative
Method	:	other
Year	:	1983
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	Negative in two trials without activation and negative in two additional trials with exogenous activation with S-9.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Reliability	:	(2) valid with restrictions Acceptable study with adequate documentation.
Reference	:	National Toxicology Program. (1983). Accessed 12/20/2004 http://ntp-apps.niehs.nih.gov/

Type	:	Sister chromatid exchange assay
System of testing	:	
Test concentrations	:	50, 160, 500, 1,600 or 5,000 µg/mL
Cytotoxic concentr.	:	
Metabolic activation	:	With and without
Result	:	negative
Method	:	other
Year	:	1983
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	Negative in two trials without activation and negative in two additional trials with exogenous activation with S-9.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP.
Reliability	:	(2) valid with restrictions Acceptable study with adequate documentation.
Reference	:	National Toxicology Program. (1983). Accessed 12/20/2004 http://ntp-apps.niehs.nih.gov/

5.6 GENETIC TOXICITY – "IN VIVO"

5.7 CARCINOGENICITY

Species	:	Rats
Strain	:	Other: F344/N
Sex	:	Male/female
Route of admin.	:	Drinking water
Exposure period	:	104 weeks (males) or 105 weeks (females)
Frequency of treatment	:	Continuous
Post exposure period	:	None
Doses	:	500, 1,250 or 2,500 ppm barium chloride dihydrate in drinking water corresponding to daily doses of 15, 30 or 60 mg Ba/kg body weight for males and 15, 45 or 75 mg Ba/kg body weight for females.
Control group	:	Yes, concurrent vehicle
Result	:	negative
Method	:	Other
Year	:	1994
GLP	:	no data
Test substance	:	As prescribed by 1.1-1.4
Method	:	60 per sex per dose; Measurements included survival, body weight, water consumption, clinical signs to toxicity, hematology, clinical chemistry and pathology. At 15 months, the plasma barium concentrations were determined. Barium levels on bone were also determined in the high dose group.
Results	:	Two-year survival was similar to controls. Final mean body weights were decreased at 2,500 ppm by 5% in males and 11% in females. Water consumption was decreased starting as early as week 5 in both sexes at the high dose. There were no clinical signs that could be related to treatment. No hematology or clinical chemistry changes were noted. In the special study at 15 months, plasma barium levels were significantly increased in males at the 1,250 and 2,500 ppm and in all treatment groups in females. Barium levels in bones of rats in the high dose group were 400 times greater than controls at the 15 month interval. There were no increases in neoplasms or non-neoplastic lesions that could be attributed to the test material. However, a dose-related increase occurred in adrenal medulla pheochromocytomas and in mononuclear cell leukemia in male rats.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP. Barium was classified as Group D (not classifiable as to human carcinogenicity) (information from EPA Integrated Risk Information System (IRIS).
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

Species	:	Mouse
Strain	:	B6C3F1
Sex	:	Male/female
Route of admin.	:	Drinking water
Exposure period	:	104 weeks (females) or 103 weeks (males)
Frequency of treatment	:	Continuous
Post exposure period	:	None

Doses	:	500, 1,250 or 2,500 ppm barium chloride dihydrate in drinking water corresponding to daily doses of 30, 75 or 160 mg Ba/kg body weight for males and 40, 90 or 200 mg Ba/kg body weight for females.
Control group	:	Yes, concurrent vehicle
Result	:	Negative
Method	:	Other
Year	:	1994
GLP	:	No data
Test substance	:	As prescribed by 1.1-1.4
Method	:	Measurements included survival, body weight, water consumption, clinical signs to toxicity, hematology, clinical chemistry and pathology. At 15 months, the plasma barium concentrations were determined.
Results	:	Two-year survival in both sexes at the high does was significantly lower than control due to renal toxicity. Final mean body weights were decreased at 2,500 ppm by 9% in males and 12% in females. Water consumption was similar to controls. There were no clinical signs that could be related to treatment. No hematology or clinical chemistry changes were noted. In the special study at 15 months, plasma barium levels were significantly increased in all exposure levels. There were no increases in neoplasms, but the incidence of hepatocellular adenoma was significantly decreased in male mice at the high dose. There was also a dose-related increase in nephropathy in both sexes.
Remark	:	Although not stated in the summary, the NTP study was likely conducted according to GLP. Barium was classified as Group D (not classifiable as to human carcinogenicity) (information from EPA Integrated Risk Information System (IRIS).
Reliability	:	(2) valid with restrictions Comparable to guideline study with adequate documentation.
Reference	:	National Toxicology Program. (Jan. 1994) Toxicology and Carcinogenesis Studies of Barium Chloride Dihydrate (CAS No. 10326-27-9) in F-344/N Rats and B6C3F1 Mice (Drinking Water Studies). TR-432.

5.8.1 TOXICITY TO FERTILITY

Type	:	One generation study
Species	:	Rat
Strain	:	Other: F344/N
Sex	:	Males/females
Route of admin.	:	Drinking water
Exposure period	:	60 days prior to mating
Frequency of treatment	:	Continuous
Premating exposure period	:	Male: 60 days Female: 60 days
Duration	:	Through delivery
Number of Gen Studies	:	One
Doses	:	1,000, 2,000 or 4,000 mg/L
Control group	:	Yes, concurrent vehicle
Result	:	
Method	:	other
Year	:	1992
GLP	:	No data
Test substance	:	other TS

Method	:	Rats were exposed for 60 days followed by an 8-day mating period. Measurements included: weekly body weight, water consumption, fertility index, fetal and maternal toxicity, developmental toxicity in fetus and neonates
Results	:	There were no indications of reproductive or developmental toxicity. However, there were below normal pregnancy rates in all groups including unexposed controls.
Remark	:	A 1977 study by Tarasenko resulted in a shortening of the estrus cycle in rats exposed to 13.4 mg of barium carbonate/m^3 for 4 months when compared to controls. This study also found an alteration in the proportion of mature and dying ovarian follicles and an increase in underdeveloped offspring that showed considerable mortality and slow weight gain during the first two post-natal months. These results were not seen at a lower dose of 3.1 mg/m^3 (summarized in WHO document)
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Sufficient experimental details present as a summary in a peer reviewed source
Reference	:	WHO Environmental Health Criteria 107, Barium (1990)

Type	:	One generation study
Species	:	Mouse
Strain	:	B6C3F1
Sex	:	Males/females
Route of admin.	:	Drinking water
Exposure period	:	60 days prior to mating
Frequency of treatment	:	Continuous
Premating exposure period	:	Male: 60 days Female: 60 days
Duration	:	Through delivery
Number of Gen Studies	:	One
Doses	:	500, 1,000 or 2,000 mg/L
Control group	:	Yes, concurrent vehicle
Result	:	
Method	:	other
Year	:	1992
GLP	:	No data
Test substance	:	other TS

Method	:	Mice were exposed for 60 days followed by an 8-day mating period. Measurements included: weekly body weight, water consumption, fertility index, fetal and maternal toxicity, developmental toxicity in fetus and neonates
Results	:	There were no indications of reproductive or developmental toxicity. However, there were below normal pregnancy rates in all groups including unexposed controls.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Sufficient experimental details present as a summary in a peer reviewed source
Reference	:	WHO Environmental Health Criteria 107, Barium (1990)

5.8.2 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species	:	rat

Sex	:	male/female
Strain	:	other: F344/N
Route of admin.	:	Drinking water
Exposure period	:	60 days prior to mating
Frequency of treatm.	:	Continuous
Duration of test	:	Through delivery
Doses	:	1,000, 2,000 or 4,000 mg/L
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	
NOAEL teratogen.	:	
Method	:	Other
Year	:	1992
GLP	:	Yes
Test substance	:	Other TS
Method	:	Rats were exposed for 60 days followed by an 8-day mating period. Measurements included weekly body weight, water consumption, fertility index, fetal and maternal toxicity, developmental toxicity in fetus and neonates.
Result	:	There was no indications of reproductive or developmental toxicity.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Sufficient experimental details present as a summary in a peer reviewed source
Reference	:	WHO Environmental Health Criteria 107, Barium (1990)
Flag	:	Critical study for SIDS endpoint

Species	:	Mouse
Sex	:	male/female
Strain	:	B6C3F1
Route of admin.	:	Drinking water
Exposure period	:	60 days prior to mating
Frequency of treatm.	:	Continuous
Duration of test	:	Through delivery
Doses	:	500, 1,000, or 2,000 mg/L
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	
NOAEL teratogen.	:	
Method	:	Other
Year	:	1992
GLP	:	Yes
Test substance	:	Other TS
Method	:	Mice were exposed for 60 days followed by an 8-day mating period. Measurements included weekly body weight, water consumption, fertility index, fetal and maternal toxicity, developmental toxicity in fetus and neonates.
Result	:	There was no indications of reproductive or developmental toxicity.
Test substance	:	Barium chloride dihydrate
Reliability	:	(2) valid with restrictions Sufficient experimental details present as a summary in a peer reviewed source
Reference	:	WHO Environmental Health Criteria 107, Barium (1990)
Flag	:	Critical study for SIDS endpoint

5.8.3 TOXICITY TO REPRODUCTION

1. General Information

ID 7727-43-7

Date 10 Nov 2005

1.0 SUBSTANCE INFORMATION

Generic Name	:	Barium sulfate
Chemical Name	:	Barium sulfate
CAS Registry No.	:	7727-43-7
Component CAS Nos.	:	
EINECS No.	:	
Structural Formula	:	$BaSO_4$
Additional description	:	Fine, heavy, odorless powder or polymorphous crystals; occurs in nature as the mineral barite
Molecular Weight	:	233.39
Synonyms and Tradenames	:	Barium sulphate; RTECS CR0600000; Radiopaque; Telebar; Microtrast; E-Z-Plaque; heavy spar, HSDB 5041, ICSC 0827
	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)
References		O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ. (molecular weight value)

2.1 MELTING POINT

Value	:	= 1580 °C
Decomposition	:	yes
Sublimation	:	
Method	:	other
Year	:	1973
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Remark	:	Data abstracted from Perry and Chilton
Reliability	:	(2) valid with restrictions Source is peer-reviewed published document.
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

2.2 BOILING POINT

Value	:	= 1149 °C (monoclinic transition point)
Decomposition	:	
Method	:	other
Year	:	1983
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Remark	:	Data abstracted from Parmeggiani
Reliability	:	(2) valid with restrictions Source is peer-reviewed published document.
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

2.3 DENSITY

Type	:	density
Value	:	= 4.50 g/cm^3
Method	:	other
Year	:	1983
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Source is peer-reviewed published document.
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

2.4 VAPOR PRESSURE

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log Pow	:	

pH value	:	
Method	:	other
Year	:	2002
GLP	:	no
Test substance	:	As prescribed by 1.1-1.4
Remark	:	Not applicable because barium sulfate is nearly insoluble in water and alcohol
Reliability	:	(2) valid with restrictions Source is well established data compendium
Reference	:	O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ. (information on solubility)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	water
Guideline/method	:	
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
PKa	:	at °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	2002
GLP	:	no
Test substance	:	As prescribed by 1.1-1.4
Result	:	Practically insoluble in water (one gram dissolves in 400,000 parts)
Reliability	:	(2) valid with restrictions Source is well established data compendium.
Reference	:	O'Neil, M.J., Smith, A., Heckelman, P.E., and J.R. Obenchain (eds.). 2002. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Ed. Merck & Co., Inc., Whitehouse Station, NJ.

2.9 FLAMMABILITY

Result	:	Non flammable
Method	:	other
Year	:	2005
Test substance	:	As prescribed by 1.1-1.4
Reliability	:	(2) valid with restrictions Data taken from a secondary literature source (electronic database)
Reference	:	http://inchem.org/documents/icsc/icsc/eics0827.htm (accessed 11/10/05)

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Year	:	2005
Test substance	:	As prescribed by 1.1-1.4
Method	:	EPIWIN
Result	:	Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.42e-006	1e+005	1000
Water	47.4	900	1000
Soil	52.5	900	1000
Sediment	0.091	3.6e+003	0

Persistence Time: 804 hr

Reliability	:	(2) valid with restrictions Data were obtained by modeling.
Reference	:	EPIWIN (ver 3.11) (2005)

3.3.2 DISTRIBUTION

3.5 BIODEGRADATION

4.1 ACUTE TOXICITY TO FISH

Type	:	
Species	:	Molly (*Poecillia latipinna.*)
Exposure period	:	96 hours
Unit	:	ug/L
NOEC	:	
LC0	:	= 59,000,000
LC50	:	
LC100	:	
Limit test	:	
Analytical monitoring	:	No data
Method	:	other
Year	:	1975
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4

Result	:	Not acutely toxic to Mollies
Remark	:	This is the only aquatic study found, probably due to the fact that barium sulfate is virtually insoluble in water (data derived from U.S. EPA, AQUIRE database, 2005)
Reliability	:	(2) valid with restrictions Although this is not a Guideline study and few experimental details are present, the results seem credible due to the physical properties of the test material. Data taken from a secondary literature source (electronic database)
Reference	:	U.S. EPA AQUIRE database, 2005 (accessed on 11/10/2005))

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	Flow-through
Species	:	Yellow Rock Crab (*Cancer anthonyi*)
Exposure period	:	7 day
NOEC	:	
EC0	:	
LC50	:	
EC100	:	
Limit test	:	
Analytical monitoring	:	No data
Method	:	other
Year	:	1978
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Flow-through; hatch and embryo
Result	:	LC50 = 10,000 (hatch) and LC50 = 100,000 µg/L (embryo); Not acutely toxic
Reliability	:	(2) valid with restrictions Although few experimental details were found, the results seem credible based on the lack of water solubility. Data taken from a secondary literature source (electronic database)
Reference	:	U.S. EPA AQUIRE database, 2005 (accessed on 11/10/05 via http://www.pesticideinfo.org/List_AquireAll.jsp?Rec_Id=PC33796&Taxa_Group=Crustaceans)
Type	:	Static
Species	:	Water flea (*Daphnia magna*)
Exposure period	:	48 Hr
Unit	:	ug/L
NOEC	:	
EC0	:	32,000 µg/L (48 Hr)
LC50	:	
EC100	:	
Limit test	:	
Analytical monitoring	:	
Method	:	other
Year	:	1989
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Result	:	24-hr EC0 = 52,820 ug/L; Not acutely toxic
Remark	:	Another study resulted in 24 and 48 hour EC50 of 4.64 and 2.81 mg/L,

respectively (Khangarot and Ray, 1989)

Reliability : (2) valid with restrictions
Comparable to a Guideline Study

Reference : U.S. EPA AQUIRE database, 2005 (accessed on 11/10/05 via http://www.pesticideinfo.org/List_AquireAll.jsp?Rec_Id=PC33796&Taxa_Group=Zooplankton)
Khangarot, B.S. and P. K. Ray. (1989) Investigation of Correlation between Physicochemical Properties of Metals and their Toxicity to the Water Flea *Daphnia magna* Straus. Ecotoxicol. Environ. Saf. 38:109-120.

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

In vitro/in vivo	:	In vivo
Type	:	Distribution
Species	:	
Number of animals	:	
Males	:	
Females	:	
Doses	:	
Males	:	
Females	:	
Vehicle	:	
Route of administration	:	
Exposure time	:	
Product type guidance	:	
Decision on results on acute tox. tests	:	
Adverse effects on prolonged exposure	:	
Half-lives	:	1st: bone Estimated to be about 50 days 2nd: 3rd:
Toxic behavior	:	
Deg. product	:	
Deg. products CAS#	:	
Method	:	Other
Year	:	2005
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4

Remark : Barium sulfate is administered as a drug either orally or rectally because it has radiopaque properties that aid in diagnostic X-ray imaging. Most of the drug is excreted in the feces within a few days and is virtually absent within two weeks. Residual amounts of barium sulfate may be retained in the bone or teeth since it can mimic calcium and be absorbed by calcified tissue. Inhaled barium sulfate dust, not cleared by ciliary action, may accumulate in the lungs in sufficient quantities to cause baritosis (benign pneumoconiosis). Barium clearance is increased by intravenous administration of saline solutions. In Sprague-Dawley rats, fasting increased the concentration of barium in the blood.

Reliability	:	(2) valid with restrictions Credible information consistent with physical properties; Data taken from a secondary literature source (electronic database)
Reference	:	Hazardous Substances Data Bank http://toxnet.nlm.nih.gov (accessed 8/16/05) http://risk.lsd.ornl.gov/tox/profiles/barium_f_V1.shtml#te (accessed 11/10/05)
In vitro/in vivo	:	In vivo
Type	:	Distribution
Species	:	Rat
Number of animals	:	
Males	:	
Females	:	
Doses	:	
Males	:	40 mg
Females	:	40 mg
Vehicle	:	
Route of administration	:	Inhalation
Exposure time	:	60 days
Product type guidance	:	
Decision on results on acute tox. tests	:	
Adverse effects on prolonged exposure	:	
Half-lives	:	1st: 2nd: 3rd:
Toxic behavior	:	
Deg. product	:	
Deg. products CAS#	:	
Method	:	Other
Year	:	1990
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Two-month inhalation exposure followed by 4 week post-exposure period
Result	:	Barium levels increased in the bones (particularly the jaw and femur), but the rate of accumulation decreased with continued exposure. The barium content in the lungs was highest two weeks after exposure initiation, but decreased over the next four weeks. However, it increased again during the following 4-week non-exposure period. No increase in barium was noted in lymph nodes.
Reliability	:	(2) valid with restrictions Results are generally consistent with other known information regarding barium metabolism. Data taken from a secondary literature source (electronic database)
Reference	:	http://toxnet.nlm.nih.gov (accessed 8/16/05)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	
Species	:	Rat
Strain	:	Other: CBL-Wistar

Sex	:	No data
Number of animals	:	
Vehicle	:	Other: Assumed to be water administered in 150% (wt/v) suspension
Doses	:	188, 225, 263, 300, 338 or 375 g/Kg
Method	:	other
Year	:	1985
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	Single dose administered intragastrically. Young rats weighing 130-160 grams were fasted for 16 hours prior to dose administration. Clinical measurements were made for 3-14 days or until death occurred.
Result	:	The interval to death decreased with increasing barium dosage.
Remark	:	The cause of death was determined to be stomach rupture due to dosing errors.
Reliability	:	(3) invalid Dosing errors confounded the study
Reference	:	USEPA Drinking Water Criteria Document for Barium (1985)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Remark	:	Not expected to cross intact skin due to the low water solubility and physical form of the test material
Reliability	:	(2) valid with restrictions Source is peer-reviewed published document.
Reference	:	ATSDR, 1992 (Agency for Toxic Substances and Disease Registry, Toxicological Profile for Barium and Compounds, July 1992)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY – "IN VITRO"

5.6 GENETIC TOXICITY – "IN VIVO"

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

5.10 EXPOSURE EXPERIENCE

Remark	:	Accidental exposure: Children had barium sulfate accidentally injected into the eye under very high pressure after cutting into the centers of certain types of golf balls. X-ray diffraction and electron probe exams identified barium sulfate in the extra-ocular tissue. Little injury resulted. Other details were not available.
Year	:	1986
CLP	:	no
Test substance	:	Barium sulfate (possibly mixed with other compounds)
Reliability	:	(3) invalid There is some question about the identity of substance involved in this accidental exposure.
Reference	:	Grant, W.M. (1986) Toxicology of the Eye. 3rd Edition. Springfield: Charles C. Thomas Publisher, p. 134

APPENDIX 2
EPIWIN SUMMARIES

```
SMILES : O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC
CHEM   :
MOL FOR: C36 H70 O4 Ba1
MOL WT : 704.28
---------------------------- EPI SUMMARY (v3.11) -------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   3.5
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   160.00

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  15.14

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  661.06  (Adapted Stein & Brown method)
    Melting Pt (deg C):  287.83  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  7.52E-014  (Modified Grain method)
    MP  (exp database):  250 deg C

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  3.589e-012
       log Kow used: 15.14 (estimated)
       melt pt used: 160.00 deg C

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  7.0428e-007 mg/L

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Neutral Organics

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :   Incomplete
   Group Method:   Incomplete
 Henrys LC [VP/WSol estimate using EPI values]:  1.991E-014 atm-m3/mole

 Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model         :   0.6291
    Non-Linear Model     :   0.0354
 Expert Survey Biodegradation Results:
    Ultimate Survey Model:   2.2395  (months      )
    Primary Survey Model :   3.3698  (days-weeks  )
 Readily Biodegradable Probability (MITI Model):
    Linear Model         :   0.1990
    Non-Linear Model     :   0.0176

 Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
   Hydroxyl Radicals Reaction:
      OVERALL OH Rate Constant =  42.9098 E-12 cm3/molecule-sec
      Half-Life =     0.249 Days (12-hr day; 1.5E6 OH/cm3)
      Half-Life =     2.991 Hrs
   Ozone Reaction:
      No Ozone Reaction Estimation
```

```
Soil Adsorption Coefficient (PCKOCWIN v1.66):
     Koc    :  9.225E+008
     Log Koc:  8.965

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
   Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
   Log BCF =  0.500  (BCF = 3.162)
      log Kow used: 15.14 (estimated)

Volatilization from Water:
   Henry LC:  1.99E-014 atm-m3/mole  (calculated from VP/WS)
   Half-Life from Model River: 7.804E+010  hours   (3.252E+009 days)
   Half-Life from Model Lake : 8.513E+011  hours   (3.547E+010 days)

Removal In Wastewater Treatment (recommended maximum 99%):
   Total removal:              94.04  percent
   Total biodegradation:        0.78  percent
   Total sludge adsorption:    93.26  percent
   Total to Air:                0.00  percent

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)        (hr)       (kg/hr)
  Air       0.0807         5.98         1000
  Water     2.32           1.44e+003    1000
  Soil      30.7           1.44e+003    1000
  Sediment  66.9           5.76e+003    0
    Persistence Time: 2.65e+003 hr
```

```
SMILES : O=C(O)CCCCCCCCCCCCCCCCC
CHEM   : Octadecanoic acid
CAS NUM: 000057-11-4
MOL FOR: C18 H36 O2
MOL WT : 284.49
------------------------------ EPI SUMMARY (v3.11) --------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):    ------
    Vapor Pressure (mm Hg) :    ------
    Henry LC (atm-m3/mole) :    ------
    Log Kow (octanol-water):    ------
    Boiling Point (deg C)  :    ------
    Melting Point (deg C)  :    ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  7.94
    Log Kow (Exper. database match) =  8.23
       Exper. Ref:  Sangster (1993)

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  382.05  (Adapted Stein & Brown method)
    Melting Pt (deg C):  132.96  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  8.31E-006  (Modified Grain method)
    MP  (exp database):  68.8 deg C
    BP  (exp database):  383 deg C
    VP  (exp database):  7.22E-07 mm Hg at 25 deg C

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  0.003512
       log Kow used: 8.23 (expkow database)
       no-melting pt equation used
     Water Sol (Exper. database match) =  0.597 mg/L (25 deg C)
        Exper. Ref:  YALKOWSKY,SH & DANNENFELSER,RM (1992)

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  0.0093429 mg/L
    Wat Sol (Exper. database match) =  0.60
       Exper. Ref:  YALKOWSKY,SH & DANNENFELSER,RM (1992)

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Surfactants-anionic-acid

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :    5.10E-005  atm-m3/mole
   Group Method:    7.39E-005  atm-m3/mole
   Exper Database: 4.76E-07  atm-m3/mole
 Henrys LC [VP/WSol estimate using EPI values]:  8.857E-004 atm-m3/mole

 Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model          :   0.7932
    Non-Linear Model      :   0.8109
 Expert Survey Biodegradation Results:
    Ultimate Survey Model:   3.2334  (weeks       )
    Primary Survey Model :   4.0919  (days        )
 Readily Biodegradable Probability (MITI Model):
    Linear Model          :   0.8380
```

Non-Linear Model : 0.9120

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 22.4804 E-12 cm3/molecule-sec
Half-Life = 0.476 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 5.710 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
Koc : 1.167E+004
Log Koc: 4.067

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
Log BCF = 1.000 (BCF = 10)
log Kow used: 8.23 (expkow database)

Volatilization from Water:
Henry LC: 4.76E-007 atm-m3/mole (Henry experimental database)
Half-Life from Model River: 2076 hours (86.51 days)
Half-Life from Model Lake : 2.279E+004 hours (949.7 days)

Removal In Wastewater Treatment (recommended maximum 99%):
Total removal: 94.02 percent
Total biodegradation: 0.78 percent
Total sludge adsorption: 93.25 percent
Total to Air: 0.00 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.676	11.4	1000
Water	7.19	360	1000
Soil	28.9	360	1000
Sediment	63.3	1.44e+003	0

Persistence Time: 640 hr

```
SMILES : [Ba]
CHEM   : BARIUM
CAS NUM: 007440-39-3
MOL FOR: Ba1
MOL WT : 137.33
---------- EPI SUMMARY (v3.11) ----------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  0.23

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  482.98  (Adapted Stein & Brown method)
    Melting Pt (deg C):  188.60  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  0  (Modified Grain method)
    MP  (exp database):  710 deg C
    BP  (exp database):  1600 deg C

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  5.476e+004
       log Kow used: 0.23 (estimated)
       no-melting pt equation used

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  2.4377e+005 mg/L

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Neutral Organics

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :   2.45E-002  atm-m3/mole
   Group Method:   Incomplete
Henrys LC [VP/WSol estimate using EPI values]:  not available

Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model         :   0.6822
    Non-Linear Model     :   0.7424
Expert Survey Biodegradation Results:
    Ultimate Survey Model:   2.8957  (weeks       )
    Primary Survey Model :   3.6496  (days-weeks  )
Readily Biodegradable Probability (MITI Model):
    Linear Model         :   0.3036
    Non-Linear Model     :   0.1917

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =   0.0000 E-12 cm3/molecule-sec
     Half-Life =   -------
  Ozone Reaction:
     No Ozone Reaction Estimation
```

Soil Adsorption Coefficient (PCKOCWIN v1.66):
Koc : 14.3
Log Koc: 1.155

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
Log BCF = 0.500 (BCF = 3.162)
log Kow used: 0.23 (estimated)

Volatilization from Water:
Henry LC: 0.0245 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 1.224 hours
Half-Life from Model Lake : 111.6 hours (4.651 days)

Removal In Wastewater Treatment (recommended maximum 99%):
Total removal: 90.51 percent
Total biodegradation: 0.02 percent
Total sludge adsorption: 0.40 percent
Total to Air: 90.09 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	37.9	1e+005	1000
Water	55.8	360	1000
Soil	6.18	360	1000
Sediment	0.0944	1.44e+003	0

Persistence Time: 180 hr

```
SMILES : O1S(=O)(=O)O[Ba]1
CHEM   : BARIUM SULFATE
CAS NUM: 007727-43-7
MOL FOR: O4 S1 Ba1
MOL WT : 233.38
---------- EPI SUMMARY (v3.11) ----------

Physical Property Inputs:
   Water Solubility (mg/L):   ------
   Vapor Pressure (mm Hg) :   ------
   Henry LC (atm-m3/mole) :   ------
   Log Kow (octanol-water):   ------
   Boiling Point (deg C)  :   ------
   Melting Point (deg C)  :   ------

Log Octanol-Water Partition Coef (SRC):
   Log Kow (KOWWIN v1.67 estimate) =  0.63

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
   Boiling Pt (deg C):  659.07  (Adapted Stein & Brown method)
   Melting Pt (deg C):  286.90  (Mean or Weighted MP)
   VP(mm Hg,25 deg C):  5.48E-019  (Modified Grain method)
   MP  (exp database):  560 dec deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):
   Water Solubility at 25 deg C (mg/L):  8470
      log Kow used: 0.63 (estimated)
      no-melting pt equation used
    Water Sol (Exper. database match) =  3.2e+004 mg/L (20 deg C)
       Exper. Ref:  SHIU,WY ET AL. (1990)

Water Sol Estimate from Fragments:
   Wat Sol (v1.01 est) =  7084.2 mg/L
   Wat Sol (Exper. database match) =  32000.00
      Exper. Ref:  SHIU,WY ET AL. (1990)

ECOSAR Class Program (ECOSAR v0.99g):
   Class(es) found:
      Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
  Bond Method :    Incomplete
  Group Method:    Incomplete
Henrys LC [VP/WSol estimate using EPI values]:  1.987E-023 atm-m3/mole

Probability of Rapid Biodegradation (BIOWIN v4.01):
   Linear Model         :   0.6364
   Non-Linear Model     :   0.4242
Expert Survey Biodegradation Results:
   Ultimate Survey Model:   2.6834  (weeks-months)
   Primary Survey Model :   3.5110  (days-weeks  )
Readily Biodegradable Probability (MITI Model):
   Linear Model         :   0.0178
   Non-Linear Model     :   0.0146

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =   0.0000 E-12 cm3/molecule-sec
```

Half-Life = -------
Ozone Reaction:
No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
Koc : 14.55
Log Koc: 1.163

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
Log BCF = 0.500 (BCF = 3.162)
log Kow used: 0.63 (estimated)

Volatilization from Water:
Henry LC: 1.99E-023 atm-m3/mole (calculated from VP/WS)
Half-Life from Model River: 4.502E+019 hours (1.876E+018 days)
Half-Life from Model Lake : 4.911E+020 hours (2.046E+019 days)

Removal In Wastewater Treatment (recommended maximum 99%):
Total removal: 1.86 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.77 percent
Total to Air: 0.00 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.42e-006	1e+005	1000
Water	47.4	900	1000
Soil	52.5	900	1000
Sediment	0.091	3.6e+003	0

Persistence Time: 804 hr

```
SMILES : CL[Ba]CL
CHEM   : Barium chloride (BaCl2)
CAS NUM: 010361-37-2
MOL FOR: Cl2 Ba1
MOL WT : 208.23
---------------------------- EPI SUMMARY (v3.11) -------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  0.85

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  515.63  (Adapted Stein & Brown method)
    Melting Pt (deg C):  205.22  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  4.42E-010  (Modified Grain method)

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  7468
       log Kow used: 0.85 (estimated)
       no-melting pt equation used

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  98484 mg/L

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Neutral Organics

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :   Incomplete
   Group Method:   Incomplete
Henrys LC [VP/WSol estimate using EPI values]:  1.622E-014 atm-m3/mole

 Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model         :   0.6484
    Non-Linear Model     :   0.5129
Expert Survey Biodegradation Results:
    Ultimate Survey Model:   2.7390  (weeks-months)
    Primary Survey Model :   3.5473  (days-weeks   )
Readily Biodegradable Probability (MITI Model):
    Linear Model         :   0.0926
    Non-Linear Model     :   0.0297

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =   0.0000 E-12 cm3/molecule-sec
     Half-Life =   -------
  Ozone Reaction:
     No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
```

Koc : 23.74
Log Koc: 1.376

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
Log BCF = 0.500 (BCF = 3.162)
log Kow used: 0.85 (estimated)

Volatilization from Water:
Henry LC: 1.62E-014 atm-m3/mole (calculated from VP/WS)
Half-Life from Model River: 5.21E+010 hours (2.171E+009 days)
Half-Life from Model Lake : 5.684E+011 hours (2.368E+010 days)

Removal In Wastewater Treatment (recommended maximum 99%):

Total removal:	1.87	percent
Total biodegradation:	0.09	percent
Total sludge adsorption:	1.78	percent
Total to Air:	0.00	percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	9.42e-006	1e+005	1000
Water	46	900	1000
Soil	53.9	900	1000
Sediment	0.0906	3.6e+003	0

Persistence Time: 813 hr

APPENDIX 1
ROBUST SUMMARIES

201-16118132

I U C L I D

Data Set

Existing Chemical	:	ID: 6865-35-6
CAS No.	:	6865-35-6
EINECS Name	:	barium distearate
EC No.	:	229-966-3
Molecular Formula	:	C18H36O2.1/2Ba

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	19.12.2005

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	19.12.2005
Status	:	
Memo	:	Barium stearate
Printing date	:	22.12.2005
Revision date	:	
Date of last update	:	21.12.2005
Number of pages	:	10
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 160 °C
Sublimation	:	
Method	:	
Year	:	1978
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Published information

19.12.2005 (1)

2.2 BOILING POINT

Value	:	= 661.1 °C at
Decomposition	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark	:	Barium stearate is a solid; determination of boiling point is not appropriate
Result	:	Boiling Pt (deg C): 661.06 (Adapted Stein & Brown method)
Test substance	:	SMILES : O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC C MOL FOR: C36 H70 O4 Ba1 MOL WT : 704.28
Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint

21.12.2005 (3)

2.4 VAPOUR PRESSURE

Value	:	= .0000000000001 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Remark	:	Barium stearate is a solid; determination of vapor pressure is not appropriate
Result	:	VP(mm Hg,25 deg C): 7.52E-014 (Modified Grain method)
Test substance	:	SMILES : O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC C MOL FOR: C36 H70 O4 Ba1 MOL WT : 704.28

Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint
21.12.2005		(2) (3)

2.5 PARTITION COEFFICIENT

Method	:	
Year	:	2002
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Determination of partition coefficient is not relevant. The substance readily dissociates.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
21.12.2005		(5)
Partition coefficient	:	octanol-water
Log pow	:	= 15.14 at °C
pH value	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	(KOWWIN v1.67 estimate)
Result	:	Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1.67 estimate) = 15.14
Test substance	:	SMILES : O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC C MOL FOR: C36 H70 O4 Ba1 MOL WT : 704.28
Reliability	:	(2) valid with restrictions Data were obtained by modeling
21.12.2005		(3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	ca. 3.5 mg/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other
Year	:	2004
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	A preliminary study was performed to determine the approximate equivalence point. As part of method development, an approximate solubility was determined

by Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES).

Reliability : (2) valid with restrictions
Not a guideline method

19.12.2005 (5)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative Intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	
Rate constant	:	= .0000000000429098 cm³/(molecule*sec)
Degradation	:	= 50 % after .3 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Result	:	Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 42.9098 E-12 cm3/molecule-sec Half-Life = 0.249 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 2.991 Hrs Ozone Reaction: No Ozone Reaction Estimation
Test substance	:	SMILES : O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC C MOL FOR: C36 H70 O4 Ba1 MOL WT : 704.28
Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint

21.12.2005 (3)

3.1.2 STABILITY IN WATER

Deg. product	:	
Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Determination of hydrolysis is not relevant. The substance readily dissociates.
Reliability	:	(2) valid with restrictions Endpoint represented using dissociation products

19.12.2005 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)

Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year : 2005

Result : Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0807	5.98	1000
Water	2.32	1.44e+003	1000
Soil	30.7	1.44e+003	1000
Sediment	66.9	5.76e+003	0

Persistence Time: 2.65e+003 hr

Test substance : SMILES :
O=C(O[Ba]OC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC
C
MOL FOR: C36 H70 O4 Ba1
MOL WT : 704.28

Reliability : (2) valid with restrictions
Data were obtained by modeling

Flag : Critical study for SIDS endpoint
21.12.2005 (3)

3.5 BIODEGRADATION

Deg. product :
Method :
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Determination of biodegradation is not relevant. The substance readily dissociates.

Reliability : (2) valid with restrictions
Endpoint represented using dissociation products

19.12.2005 (5)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Based on the low water solubility of barium stearate, ready dissociation, and high partition coefficient of stearic acid, acute aquatic toxicity testing is not appropriate.
Reliability	:	(2) valid with restrictions Based on the physical/chemical properties of the substance

19.12.2005 (5)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Based on the low water solubility of barium stearate, ready dissociation, and high partition coefficient of stearic acid, acute aquatic toxicity testing is not appropriate.
Reliability	:	(2) valid with restrictions Based on the physical/chemical properties of the substance

19.12.2005 (5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Based on the low water solubility of barium stearate, ready dissociation, and high partition coefficient of stearic acid, acute aquatic toxicity testing is not appropriate.
Reliability	:	(2) valid with restrictions Based on the physical/chemical properties of the substance

19.12.2005 (5)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	3390 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions

19.12.2005 (2)

Type	:	LD50
Value	:	2506 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1992
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Published information

19.12.2005 (4)

Type	:	LD50
Value	:	1832 - mg/kg bw
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1992
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Published information

19.12.2005 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

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I U C L I D

Data Set

Existing Chemical	:	ID: 57-11-4
EINECS Name	:	stearic acid
EC No.	:	200-313-4
Molecular Formula	:	C18H36O2

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	04.12.2003

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	04.12.2003
Status	:	
Memo	:	SOCMA MCC
Printing date	:	22.12.2005
Revision date	:	
Date of last update	:	22.12.2005
Number of pages	:	12
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 69 - 70 °C
Sublimation	:	
Method	:	
Year	:	1982
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
Flag	:	Critical study for SIDS endpoint

04.12.2003 (17)

2.2 BOILING POINT

Value	:	= 383 °C at 1013 hPa
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
Flag	:	Critical study for SIDS endpoint

04.12.2003 (17)

2.4 VAPOUR PRESSURE

Value	:	= 1.33 hPa at 173.7 °C
Decomposition	:	
Method	:	
Year	:	1969
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
Flag	:	Critical study for SIDS endpoint

04.12.2003 (16)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 8.42 at °C
pH value	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

04.12.2003 (10)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= .568 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: measured
Year	:	1966
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Water solubility = .0001 mg/L at 30 deg C
Reliability	:	(2) valid with restrictions information taken from a peer-reviewed publication.

05.12.2003 (13)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	= .5 day(s)
Degradation	:	% after
Quantum yield	:	
Deg. product	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Estimated using AopWin v1.91
Result	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 22.4804 E-12 cm3/molecule-sec Half-Life = 0.476 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 5.710 Hrs Ozone Reaction: No Ozone Reaction Estimation
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.12.2005 (4)

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	= 17 hour(s)
Degradation	:	% after
Quantum yield	:	
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor phase stearic acid is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals with a half-life of about 17 hours.
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

05.12.2003 (1) (3) (7) (11)

3.1.2 STABILITY IN WATER

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: modeling
Year	:	2003
Method	:	EPI v3.11
Result	:	Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 0.676 11.4 1000 Water 7.19 360 1000 Soil 28.9 360 1000 Sediment 63.3 1.44e+003 0 Persistence Time: 640 hr
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.12.2005 (4)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	= 77 (±) % after 28 day(s)
Result	:	readily biodegradable
Kinetic of testsubst.	:	10 day(s) = 65 % 14 day(s) = 69 % 28 day(s) = 77 % % %
Deg. product	:	
Method	:	other: BOD test
Year	:	1983
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Results are an average of 11 participating laboratories.
Result	:	65, 69 and 77 % degradation after 10, 14 and 28 days, respectively.
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

22.12.2005 (8)

Type	:	aerobic
Inoculum	:	activated sludge
Concentration	:	100 g/l related to Test substance related to
Contact time	:	5 day(s)
Degradation	:	(±) % after
Result	:	readily biodegradable
Deg. product	:	
Method	:	other: BOD5
Year	:	1985
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Result	:	Rate: .0088 1/HR Half-Life [Days]: 3.3
Test condition	:	BOD test conducted at 20 deg C.
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
22.12.2005		(15)
Type	:	aerobic
Inoculum	:	other: sewage sludge
Contact time	:	21 day(s)
Degradation	:	= 95 (±) % after 21 day(s)
Result	:	readily biodegradable
Deg. product	:	
Method	:	other: Sturm CO2 evolution
Year	:	1984
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
Flag	:	Critical study for SIDS endpoint
22.12.2005		(14)
Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	(±) % after
Result	:	readily biodegradable
Deg. product	:	
Method	:	other: Warburg
Year	:	1973
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Rate: .0077; .0052; .00217 Rate Units: 1/HR Half-Life [Days]: 3.75; 5.55; 10.7
Test condition	:	Test Method: WARBURG Oxygen Condition: AEROBIC Analysis Method: 02 UPTAKE Inoculum: ACTIVATED SLUDGE Temperature [øC]: 20; 25; 30
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.
22.12.2005		(12)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period	:	96 hour(s)
Unit	:	µg/l
LC50	:	= 12000 measured/nominal
Method	:	
Year	:	1977
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	"pure"
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.12.2005 (9)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 4600 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

22.12.2005 (2)

Type	:	LD100
Value	:	= 14286 - mg/kg bw
Species	:	human
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1976
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Minimum/Potential Fatal Human Dose: 1. 1= PRACTICALLY NONTOXIC: PROBABLE ORAL LETHAL DOSE (HUMAN) MORE THAN 1 QT (2.2 LB) FOR 70 KG PERSON (150 LB).
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

22.12.2005 (5)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	
Strain	:	
Route of admin.	:	oral feed

Exposure period	:	24 weeks
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	50g/kg/day
Control group	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time.
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

22.12.2005 (2)

Type	:	Sub-acute
Species	:	rat
Sex	:	
Strain	:	
Route of admin.	:	oral feed
Exposure period	:	6 or 9 weeks
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	5 or 6%
Control group	:	
Result	:	Rats fed 5% stearic acid as part of a high-fat diet for 6 weeks, or 6% stearic acid for 9 weeks, showed a decreased blood clotting time and hyperlipemia.
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.

22.12.2005 (2)

Type	:	Sub-acute
Species	:	mouse
Sex	:	
Strain	:	
Route of admin.	:	oral feed
Exposure period	:	3 weeks
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	5 to 50%
Control group	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	When diets containing 5 to 50% stearic acid (as the monoglyceride) were fed to weanling mice for 3 weeks, depression of weight gain was seen above the 10% dietary level. Mortality occurred only with the 50% diet. The effects were less noticeable in adult mice.

Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

22.12.2005 (2)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

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I U C L I D

Data Set

Existing Chemical	:	ID: 7440-39-3
CAS No.	:	7440-39-3
EINECS Name	:	barium
EC No.	:	231-149-1
Molecular Formula	:	Ba

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	19.12.2005

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	19.12.2005
Status	:	
Memo	:	Barium
Printing date	:	22.12.2005
Revision date	:	
Date of last update	:	22.12.2005
Number of pages	:	8
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 710 °C
Sublimation	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Published information
Flag	:	Critical study for SIDS endpoint

19.12.2005 (4)

2.2 BOILING POINT

Value	:	ca. 1600 °C at
Decomposition	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Published information
Flag	:	Critical study for SIDS endpoint

19.12.2005 (4)

2.4 VAPOUR PRESSURE

Decomposition	:	
Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Not relevant based on nature of substance (metal)
Reliability	:	(2) valid with restrictions Based on physical property of substance
Flag	:	Critical study for SIDS endpoint

19.12.2005

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	.23 at 25 °C
pH value	:	
Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Log Kow (KOWWIN v1.67 estimate)
Remark	:	Not relevant based on nature of substance (metal)

Value based on Epiwin model
Reliability : (2) valid with restrictions
Data were obtained by modeling; based on physical property of substance
Flag : Critical study for SIDS endpoint
19.12.2005 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Not relevant based on nature of substance (metal)
Reliability	:	(2) valid with restrictions Based on physical property of substance
Flag	:	Critical study for SIDS endpoint

19.12.2005

3.1.1 PHOTODEGRADATION

Deg. product	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Remark	:	Cannot be modeled with Epiwin
Result	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0.0000 E-12 cm3/molecule-sec Half-Life = ------ Ozone Reaction: No Ozone Reaction Esti
Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint

22.12.2005 (1)

3.1.2 STABILITY IN WATER

Deg. product	:	
Method	:	
Year	:	2005
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Not relevant based on nature of substance (metal)
Result	:	Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]: Rate constants can NOT be estimated for this structur
Reliability	:	(2) valid with restrictions Data were obtained by modeling; Based on physical property of substance

22.12.2005 (1)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	2005
Method	:	EPI SUMMARY (v3.11)
Result	:	Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	37.9	1e+005	1000

Water	55.8	360	1000	
Soil	6.18	360	1000	
Sediment	0.0944	1.44e+003	0	

Persistence Time: 180 hr

Reliability : (2) valid with restrictions
Data were obtained by modeling

Flag : Critical study for SIDS endpoint
22.12.2005 (1)

3.5 BIODEGRADATION

Contact time :
Degradation : (±) % after
Result : other: not biodgradable
Deg. product :
Method :
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Not relevant based on nature of substance (metal)
Reliability : (2) valid with restrictions
Based on physical property of substance

Flag : Critical study for SIDS endpoint
19.12.2005

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Cyprinodon variegatus (Fish, estuary, marine)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 500
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	other TS
Test substance	:	Barium (unclear which form of barium was tested)
Reliability	:	(2) valid with restrictions 2 (Reliable with restrictions): Insufficient details are present to indicate whether all test methods followed the Guidelines. However, methods and number of studies with similar results seem sufficient to accept the data

19.12.2005 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	flow through
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	68
EC50	:	410 -
Method	:	
Year	:	1980
GLP	:	no data
Test substance	:	other TS
Result	:	>530 mg/L (at 24 hours) and 48 hour LC50 was 410 mg/L with confidence limits of 320-530 mg/L
Test substance	:	Barium (unclear which form of barium was tested)
Reliability	:	(2) valid with restrictions 2 (reliable with restrictions): Comparable to guideline study with adequate documentation.

19.12.2005 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

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